REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*
Nov 2014

2. REPORT TYPE
Viewgraph

3. DATES COVERED *(From - To)*
Nov 2014- Dec 2014

4. TITLE AND SUBTITLE
Advanced Multifluid and Collisional-Radiative models for Laser-Plasma Interaction

5a. CONTRACT NUMBER
In-house

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)
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5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER
Q02Z

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Air Force Research Laboratory (AFMC)
AFRL/RQRS
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8. PERFORMING ORGANIZATION REPORT NO.

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)
Air Force Research Laboratory (AFMC)
AFRL/RQR
5 Pollux Drive
Edwards AFB CA 93524-7048

10. SPONSOR/MONITOR'S ACRONYM(S)

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
AFRL-RQ-ED-VG-2014-363

12. DISTRIBUTION / AVAILABILITY STATEMENT
Distribution A: Approved for Public Release; Distribution Unlimited.

13. SUPPLEMENTARY NOTES
Briefing Charts presented at Plasma and Electroenergetics Program Review, Arlington, CA, 18-19 December 2014. PA#14613

14. ABSTRACT
N/A

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
					Jean-Luc Cambier
a. REPORT	b. ABSTRACT	c. THIS PAGE			19b. TELEPHONE NO *(include area code)*
Unclassified	**Unclassified**	**Unclassified**	SAR	23	661-275-5649

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std. 239.18

Advanced Multifluid and Collisional-Radiative models for Laser-Plasma Interaction

AFOSR Plasma and Electroenergetics Review Meeting
December 2014

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TOC

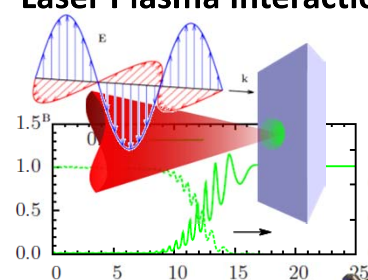
Spacecraft Plasma M&S

- **Applications: Hall thrusters, FRC, LIBS, Laser Plasma Interaction, Plasma Discharges**
- **Complex physics: excitation/ionization, transport, radiation, material, etc.**
- **Multiple spatial-temporal and density scales.**

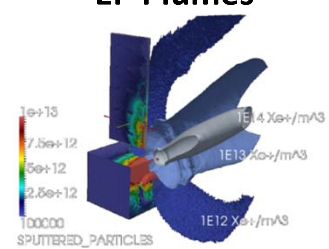
Current focus:

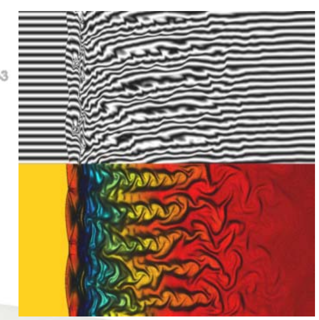
Develop advanced multiscale algorithms for plasma M&S in highly non-equilibrium condition and with collisional-radiative kinetics

Laser Plasma Interaction

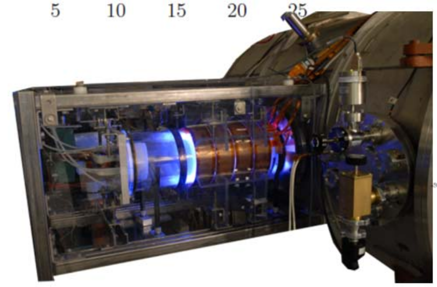


EP Plumes

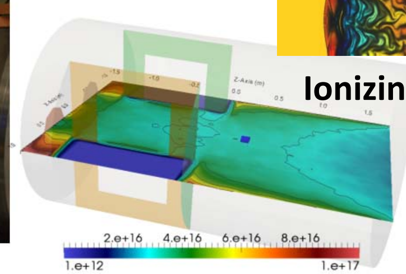




Ionizing shocks



FRC



Chamber Environment

Plasma M&S

- **Kinetic equation:**

$$\partial_t f + \vec{v}\cdot\nabla_{\vec{x}} f = \frac{1}{\varepsilon} Q(f,f) + Q^{CR}(f,f)$$

Boltzmann Coll. Op.: $$Q(f,f) = \int_{R^3}\int_{S^2} \sigma\left(|v-v_*|,\omega\right)\left[f(v')f(v_*') - f(v)f(v_*)\right]d\omega dv'$$

Equilibrium vdf: $$Q(f,f)=0 \rightarrow f(v) = \frac{\rho}{(2\pi T)^{3/2}}\exp\left(-\frac{|v-u|^2}{2T}\right)$$

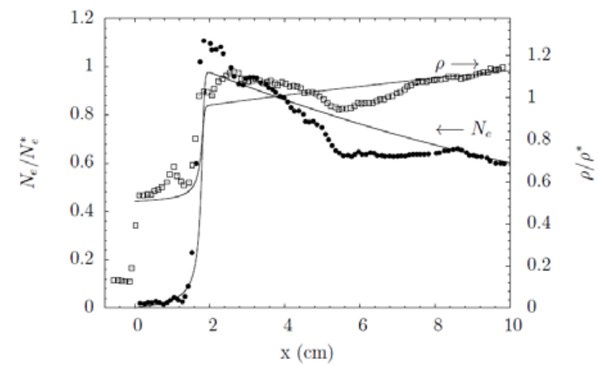
  - Fluid regime: $\varepsilon << 1$
  - Kinetic regime: $\varepsilon = O(1)$
  - Collisional plasma: excitation/ionization, CE collisions, radiation, etc.

- **Methods: moment method, PIC, DNS.**

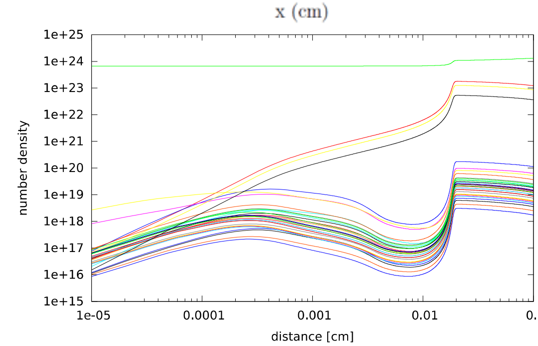
- **Challenges:**
  - Multiple species: $f \rightarrow f_s \quad Q(f,f) \rightarrow \sum_t Q(f_s, f_t)$
  - Dynamical regime: $\varepsilon \rightarrow \varepsilon(p,x,t)$

Collisional-Radiative (CR) model

- **Non-equilibrium modeling of the atomic state distribution function (ASDF)**
  - Detailed state-to-state model of atomic transition, i.e., excitation, ionization, line radiation, etc.
  - Rates derived based on ab initio cross section.
- **Examples: hypersonic shocks in Ar & N_2**
- **Complications:**
  - Accuracy can require many states
  - Translational nonequilibrium



Atomic CR
Ar shock (31 levs)



Maxwellian CR

- **Hydrogen model:** $E_n = I_H\left(1 - 1/n^2\right) \quad I_n = I_H / n^2 \quad g_n = n^2$
- **Analytical rates:**
  - Excitation/deexcitation:

$$\alpha^e_{(m|n)} \simeq \left[4\pi a_0^2 \cdot \frac{32}{\pi\sqrt{3}} \cdot \bar{v}_e\right] \frac{e^{-x_{nm}}}{n^5 m^3 (n^{-2} - m^{-2})^5},$$

$$\beta^e_{(n|m)} \simeq \left[4\pi a_0^2 \cdot \frac{32}{\pi\sqrt{3}} \cdot \bar{v}_e\right] \frac{1}{n^3 m^5 (n^{-2} - m^{-2})^5}.$$

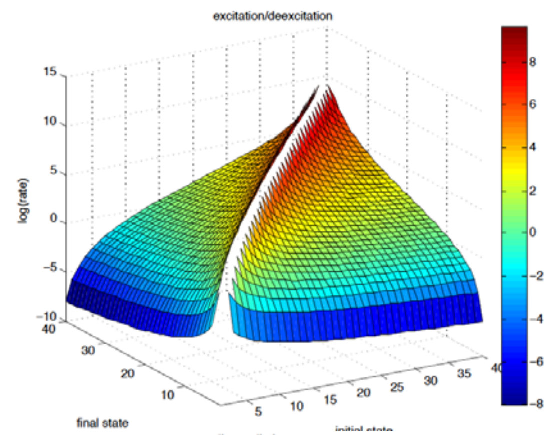
  - Ionization/recombination:

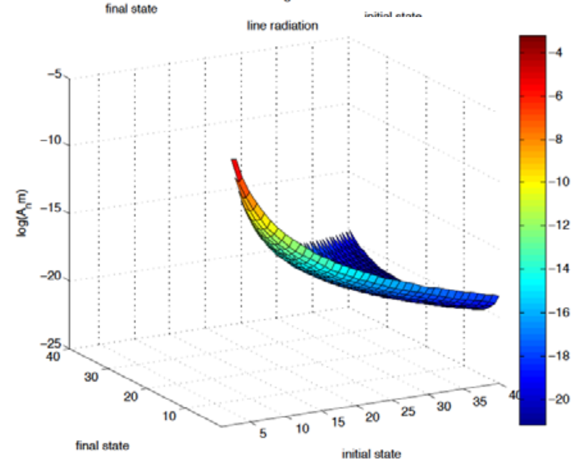
$$\alpha^e_{(+|n)} \simeq (4\pi a_0^2)\left(\frac{8kT_e}{\pi m_e}\right)^{1/2} n^4 e^{-x_n}$$

$$\beta^e_{(n|+)} \simeq \left[\frac{4}{\pi}\frac{a_0^2 h^3}{m_e^2 k T_e}\right] n^6$$

  - Line radiation

$$A_{(n|m)} = \left(\frac{8\pi^2 e^2}{m_e c^3}\right)\frac{g_n}{g_m} \mathrm{f}_{nm} = \frac{1.6 \times 10^{10}}{m^3 n (m^2 - n^2)} \mathrm{s}^{-1}$$





- **Rate equation:**

$$\frac{dN_n}{dt} = -\sum_{m>n} \alpha_{(m|n)} N_e N_n + \sum_{m>n} \beta_{(n|m)} N_e N_m + \sum_{m>n} A_{(n|m)} N_m + \sum_{m<n} \alpha_{(n|m)} N_e N_m - \sum_{m<n} \beta_{(m|n)} N_e N_n - \sum_{m<n} A_{(m|n)} N_n - \alpha_{(+|n)} N_e N_n + \beta_{(n|+)} N_+ N_e^2. \quad (8)$$

$$\frac{dN_+}{dt} = \sum_n \alpha_{(+|n)} N_e N_n - \sum_n \beta_{(n|+)} N_+ N_e^2.$$

Level grouping

- **CR modeling: level-grouping** ➡ $\mathcal{N}_n = N_{n_0}\sum_{i\in n}\frac{N_i}{N_{n_0}} \simeq \frac{N_{n_0}}{g_{n_0}}\underbrace{\sum_{i\in n} g_i e^{-\Delta E_i/T_n}}_{\mathcal{Z}_n}$
  - Group effective rates of change

$$\frac{d\mathcal{N}_n}{dt} = -N_e\mathcal{N}_n\left[\sum_{m>n}\sum_{i\in n}\frac{g_i e^{-\Delta E_i/T_n}}{\mathcal{Z}_n}\sum_{j\in m}\alpha_{(j|i)} + \sum_{m<n}\sum_{i\in n}\frac{g_i e^{-\Delta E_i/T_n}}{\mathcal{Z}_n}\sum_{j\in m}\beta_{(j|i)}\right]$$

  - Internal structure of group is assumed Boltzmann (T_n)
    – Piecewise exponential
  - This does NOT mean the entire ASDF is Boltzmann!!
  - Group temperature must be determined ➡ additional conservation equation, e.g.: $\frac{d\mathcal{E}_n}{dt} = -N_e\mathcal{N}_n\left[\sum_{m>n}\sum_{i\in n}\frac{g_i e^{-\Delta E_i/T_n}}{\mathcal{Z}_n}\sum_{j\in m}E_i\alpha_{(j|i)} + \sum_{m<n}\sum_{i\in n}\frac{g_i e^{-\Delta E_i/T_n}}{\mathcal{Z}_n}\sum_{j\in m}E_i\beta_{(j|i)}\right]$
  - Procedure?
    – Solve: $\langle\Delta E\rangle_n(\boxed{T_n^\bullet}) + C_v(\boxed{T_n^\bullet})\delta T_n^\bullet = \boxed{\frac{\Delta\mathcal{E}_n^{(k)}}{\mathcal{N}_n^{(k)}}}$ with: $\Delta\mathcal{E}_n = \sum_{i\in n}(E_i - E_{n_0})N_i = \mathcal{N}_n\boxed{\langle\Delta E\rangle_n}$, $\boxed{C_v(T_n)} = \frac{d}{dT_n}\langle\Delta E\rangle_n$

iterated

computed

tabulated

    – **However…** $\langle\Delta E\rangle_n \simeq o(\epsilon)$, $C_v(T_n) \simeq o(\epsilon)$ where $\epsilon = e^{-\Delta E_1/T_n}$ ➡ $\delta T_n^\bullet = o(\epsilon)/o(\epsilon)$

Level grouping

- **CR modeling: level-grouping**
  - Other approaches?
    - Sub-partitioning: lowest level n_0 and total $\mathcal{N}_n$ (no need for $\mathcal{E}_n$)

$$\delta T_n^\bullet \simeq \frac{T_n^{\bullet 2}}{\mathcal{Z}_n(T_n^\bullet)\langle\Delta E\rangle_n(T_n^\bullet)}\left[\frac{\mathcal{N}_n^{(k)}}{N_{n_0}^{(k)}} g_{n_0} - \mathcal{Z}_n(T_n^\bullet)\right] \quad = o(\epsilon)/o(\epsilon) \text{ ...fails}$$

    - Sub-partitioning: lowest level n_0 and upper distribution $\mathcal{N}_{n'}$

$$\delta T_n^\bullet \simeq \frac{T_n^{\bullet 2}}{\mathcal{Z}_n'(T_n^\bullet)\langle\Delta E\rangle_n(T_n^\bullet)}\left[\frac{\mathcal{N}_n^{\prime(k)}}{N_{n_0}^{(k)}} g_{n_0} - \mathcal{Z}_n'(T_n^\bullet)\right] \quad = o(\epsilon)/o(\epsilon) \text{ ...fails}$$

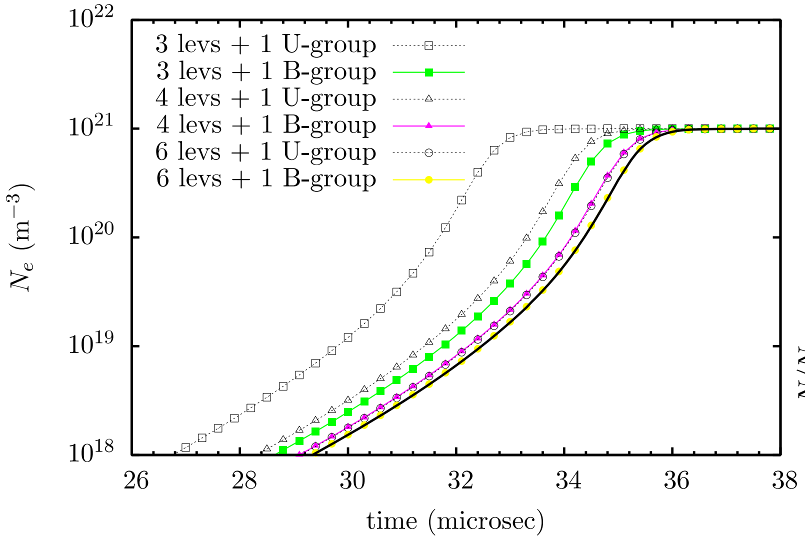
    - Approximate $\mathcal{Z}_n$ by expanding around mean energy: $\overline{\Delta E}_n = \frac{1}{g_n}\sum_{i\in n} g_i \Delta E_i$.

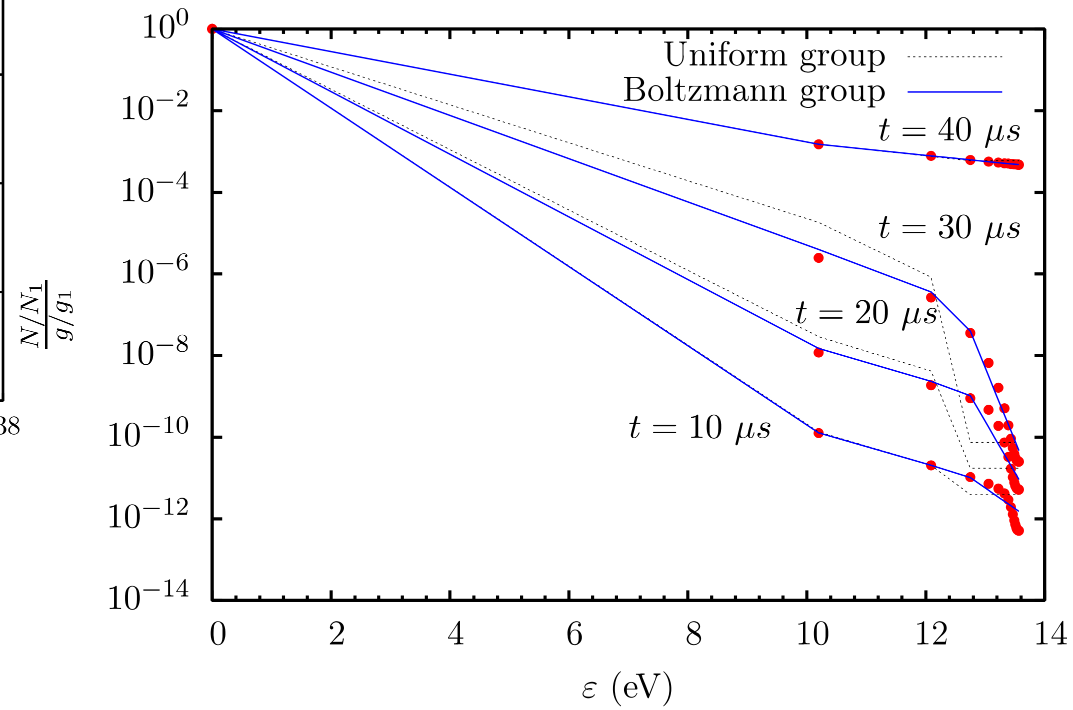
$$\mathcal{Z}_n(T_n) = e^{-\overline{\Delta E}_n/T_n}\sum_{i\in n} g_i\left[1 - \cancel{\frac{\delta_i}{T_n}} + \frac{1}{2}\frac{\delta_i^2}{T_n^2} + \dots\right] \qquad \text{where } \delta_i \equiv \Delta E_i - \overline{\Delta E}_n$$

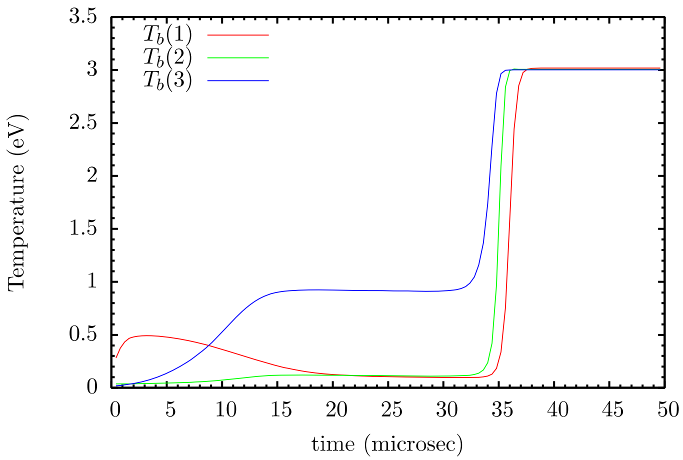
      - With n_0, $\mathcal{N}_n$ partitioning: $1/\ln(1+\varepsilon)$ ...fails
      - With n_0, $\mathcal{N}_{n'}$ partitioning: $1/\ln(\varepsilon)$ ...succeeds!
        - Improve with successive iterations… $\mathcal{Z}_n'(T_n) = \bar{g}_n'(T_n)e^{-\overline{\Delta E'}/T_n}$

Level grouping: Numerical test

- **Isothermal heat bath:**







Works very well (also tested in cooling regime).
Much better than uniform (standard) grouping.

Level grouping: Energy conservation

- **Energy conservation:**
  - Conservation follows from definition $\mathcal{E}_n = \bar{E}_n \mathcal{N}_n$
  - Start with:

$$\frac{d\Delta\mathcal{E}_n}{dt} \equiv \sum_{i \in n} \Delta E_i \frac{dN_i}{dt} = \frac{d}{dt}\left(\mathcal{N}'_n \langle \Delta E \rangle_{n'}\right) = \langle \Delta E \rangle_{n'} \boxed{\frac{d\mathcal{N}'_n}{dt}} + \mathcal{N}'_n \boxed{\frac{d\langle \Delta E \rangle_{n'}}{dt}}$$

Δ(overall group population) : $\mathcal{N}_n$

Δ(internal structure) := $C_{v,n'} \frac{dT_n}{dt}$

  - Express in terms of conserved variables:

$$\frac{d\mathcal{E}_n}{dt} = [E_{n_0} - \omega_{n'}] \frac{dN_{n_0}}{dt} + [E_{n_0} + \langle \Delta E \rangle_{n'} + \xi_{n'}] \frac{d\mathcal{N}'_n}{dt}$$

with $\xi_{n'} = \frac{C_{v,n'} T_n^2}{\left(\overline{\Delta E'}_n + T_n^2 \frac{d \ln \tilde{g}_n}{dT_n}\right)}$ and $\omega_{n'} = \xi_{n'} \frac{\mathcal{N}_{n'}}{N_{n_0}}$

Level grouping: Energy conservation

- **Energy conservation:**
  - Finally…Procedure shown to be equivalent to replacing energies by “effective” (condition-dependent) values (≈ EOS)

Excitation:

$$\bar{\alpha}^E_{(m_o|n_o)} = \left(\bar{E}_{m_o} - \bar{E}_{n_o}\right) \cdot \bar{\alpha}_{(m_o|n_o)}$$
$$\bar{\alpha}^E_{(m'|n_o)} = \left(\bar{E}_{m'} - \bar{E}_{n_o}\right) \cdot \bar{\alpha}_{(m'|n_o)}$$
$$\bar{\alpha}^E_{(m_o|n')} = \left(\bar{E}_{m_o} - \bar{E}_{n'}\right) \cdot \bar{\alpha}_{(m_o|n')}$$
$$\bar{\alpha}^E_{(m'|n')} = \left(\bar{E}_{m'} - \bar{E}_{n'}\right) \cdot \bar{\alpha}_{(m'|n')}$$

Ionization:

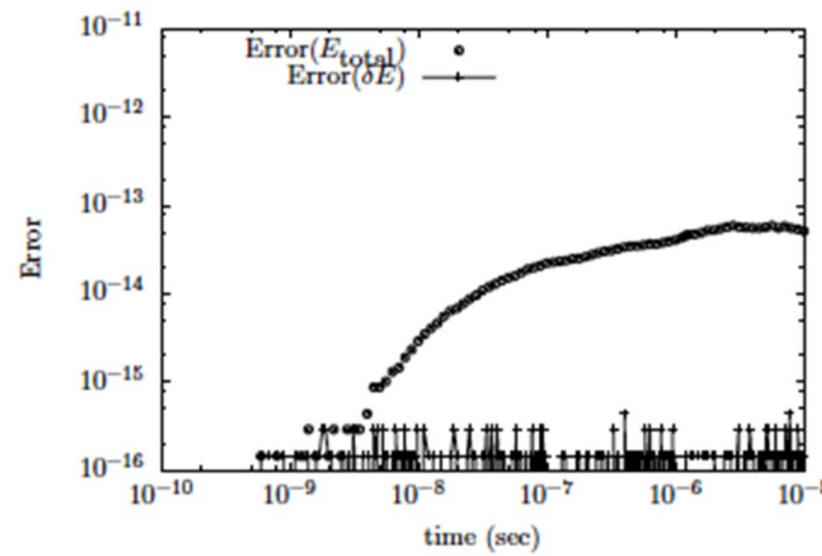
$$\bar{\alpha}^E_{(+|n_o)} = \left(I_H - \bar{E}_{n_o}\right) \cdot \bar{\alpha}_{(+|n_o)}$$
$$\bar{\alpha}^E_{(+|n')} = \left(I_H - \bar{E}_{n'}\right) \cdot \bar{\alpha}_{(+|n')}$$

with

$$\bar{E}_{n_o} = E_{n_o} - \omega_{n'}$$
$$\bar{E}_{n'} = E_{n_o} + \langle \Delta E \rangle_{n'} + \xi_{n'}$$

- **NOW**, energy is conserved

  (down to round-off)



Multi-fluid equations

- **Multi-fluid model:**
  - 5-moment:

$$\partial_t \rho_s + \nabla \cdot (\rho_s \mathbf{u}_s) = \omega_s^\rho$$

$$\partial_t(\rho_s \mathbf{u}_s) + \nabla \cdot (\rho_s \mathbf{u}_s \mathbf{u}_s + \mathbb{P}_s) = Z_s e n_s (\mathbf{E} + \mathbf{u}_s \times \mathbf{B}) + \mathbf{f}_s^m$$

$$\partial_t \varepsilon_s + \nabla \cdot (\mathbf{u}_s \varepsilon_s + \mathbb{P}_s \cdot \mathbf{u}_s) + \nabla \cdot \mathbf{q}_s = \mathbf{j}_s \cdot \mathbf{E} + \omega_s^\varepsilon$$

  - Add Maxwell's equations:

$$\nabla \times \mathbf{E} = -\partial_t \mathbf{B} \qquad \nabla \cdot \mathbf{E} = \frac{e}{\varepsilon_0}(Z_\mathrm{i} n_\mathrm{i} - n_\mathrm{e})$$

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{j} - \frac{1}{c^2}\partial_t \mathbf{E} \qquad \nabla \cdot \mathbf{B} = 0$$

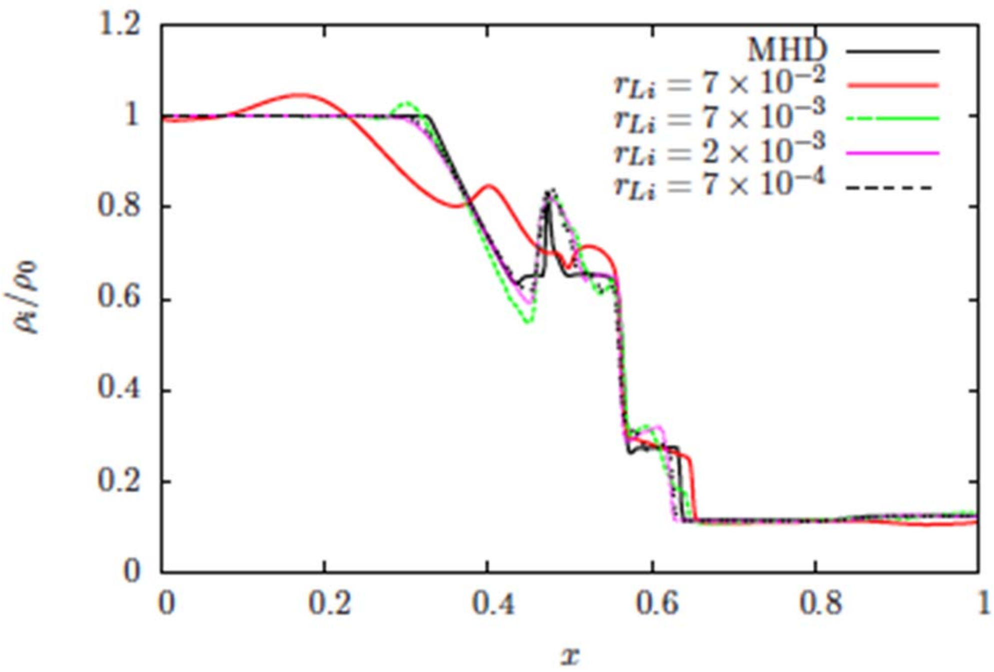
  - Add collisions:
    – Elastic – Braginskii terms
    – Inelastic – Rates depend on both T and relative velocity

$$k_i = n_\mathrm{n} n_\mathrm{e} \int\int f_\mathrm{n} f_\mathrm{e} g \sigma_i''(g; \Omega_1, \Omega_2) d\Omega_1 d\Omega_2 d^3 v_\mathrm{n} d^3 v_\mathrm{e} \quad \Rightarrow \quad k_i = k_i(T_e, |\mathbf{u}_\mathrm{n} - \mathbf{u}_\mathrm{e}|)$$

    – Multi-fluid CR model from fundamental principles being developed (incl. detailed balance)

Multi-fluid equations

- **Electromagnetic shock: generalized Brio-Wu[1]**
  - FV with WENO reconstruction and RK3



[1]Shumlak & Loverich, JCP 2003

Two-Fluid model

- **Assume fully ionized plasma, electrostatic field:**

$$\partial_t \rho_e + \nabla \cdot (\rho_e \mathbf{u}_e) = 0$$

$$\partial_t \rho_i + \nabla \cdot (\rho_i \mathbf{u}_i) = 0$$

$$\partial_t (\rho_e \mathbf{u}_e) + \nabla \cdot (\rho_e \mathbf{u}_e \mathbf{u}_e + p_e \mathbb{I}) = -e n_e \mathbf{E} + \rho_e \nu_{ei} \mathbf{w}_{ei} + \mathbf{f}_p$$

$$\partial_t (\rho_i \mathbf{u}_i) + \nabla \cdot (\rho_i \mathbf{u}_i \mathbf{u}_i + p_i \mathbb{I}) = Z_i e n_i \mathbf{E} - \rho_e \nu_{ei} \mathbf{w}_{ei}$$

$$\partial_t E_e + \nabla \cdot [(E_e + p_e)\mathbf{u}_e] = -\nabla \cdot \mathbf{q}_e + \mathbf{j}_e \cdot \mathbf{E} + \rho_e \nu_{ei} \mathbf{w}_{ei} \cdot \overline{\mathbf{u}}_{ei}$$
$$+ 3 n_e \nu_{ei} k (T_i - T_e) + \mathbf{f}_p \cdot \mathbf{u}_e + W_L$$

$$\partial_t E_i + \nabla \cdot [(E_i + p_i)\mathbf{u}_i] = \mathbf{j}_i \cdot \mathbf{E} - \rho_e \nu_{ei} \mathbf{w}_{ei} \cdot \overline{\mathbf{u}}_{ei} - 3 n_e \nu_{ei} k (T_i - T_e)$$

- **Gauss's law for electrostatic field** $\nabla \cdot \mathbf{E} = \frac{e}{\epsilon_0}(Z_i n_i - n_e)$

- **Transport: Spitzer with flux limiter**

$$\mathbf{q}_e = \min(f \frac{q_{FS}}{|\mathbf{q}_{SH}|}\mathbf{q}_{SH}, \mathbf{q}_{SH}) \qquad \kappa_e = \frac{\gamma_Z n_e k^2 T_e}{m_e \nu_{ei}}$$

$$\mathbf{q}_{SH} = -\kappa_e \nabla T_e \qquad \gamma_Z \approx \frac{3.22554(Z_i + 0.24)}{1 + 0.24 Z_i}$$

$$q_{FS} = \left(\tfrac{2}{\pi}\right)^{1/2} k T_e v_{Te}$$

Electrodynamics

- **Maxwell's equations for laser E and B fields (different from plasma)**

$$\partial_{tt}\mathbf{E} - c^2\nabla^2\mathbf{E} + c^2\nabla(\nabla\cdot\mathbf{E}) + \frac{1}{\epsilon_0}\partial_t\mathbf{j} = 0$$
$$\partial_{tt}\mathbf{B} - c^2\nabla^2\mathbf{B} - \frac{1}{\epsilon_0}\nabla\times\mathbf{j} = 0$$

- **Cold plasma response via Ohm's law:** $$\partial_t\mathbf{j} + \nu\mathbf{j} = \epsilon_0\omega_p^2\mathbf{E}$$

- **Assuming monochromatic wave:**

$$\mathbf{E}(\mathbf{x},t) = \hat{\mathbf{E}}(\mathbf{x})e^{-i\omega t} + c.c.$$
$$\mathbf{B}(\mathbf{x},t) = \hat{\mathbf{B}}(\mathbf{x})e^{-i\omega t} + c.c.$$
$$\mathbf{j}(\mathbf{x},t) = \hat{\mathbf{j}}(\mathbf{x})e^{-i\omega t} + c.c.$$

$$\hat{\mathbf{j}} = \sigma\hat{\mathbf{E}}$$

$$\sigma = \frac{i\epsilon_0\omega_p^2}{\omega(1+i\nu/\omega)}$$

Complex conductivity

Dielectric function

$$\varepsilon = \eta^2 = 1 - \frac{\omega_p^2}{\omega^2(1+i\nu/\omega)}$$

Refractive index

- **Wave equations becomes:**

$$\nabla^2\hat{\mathbf{E}} + k_0^2\varepsilon\hat{\mathbf{E}} - \nabla(\nabla\cdot\hat{\mathbf{E}}) = 0$$
$$\nabla^2\hat{\mathbf{B}} + k_0^2\varepsilon\hat{\mathbf{B}} + \nabla(\ln\varepsilon)\times\left(\nabla\times\hat{\mathbf{B}}\right) = 0$$

Ponderomotive force and collisional heating

- **Nonlinear force (Hora, *PoF* 1985)**
  - General: $\mathbf{f}_{nl} = \mathbf{j}\times\mathbf{B} + \epsilon_0 \mathbf{E}\nabla\cdot\mathbf{E} + \epsilon_0\left(1+\omega^{-1}\partial_t\right)\nabla\cdot(\eta^2-1)\mathbf{E}\mathbf{E}$
  - Assume steady-state and time-average: ponderomotive force

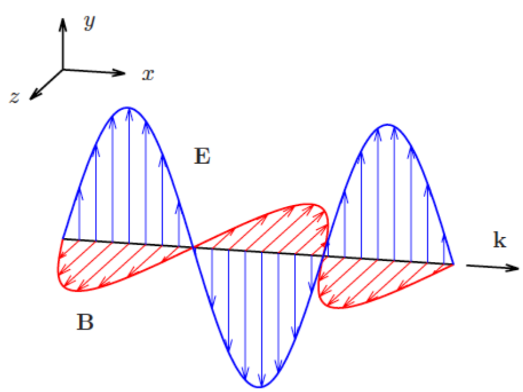
$$\mathbf{f}_p = \langle \mathbf{f}_{nl}\rangle = -\nabla\cdot\left[\langle \mathbb{T}\rangle - \epsilon_0\left(\eta^2-1\right)\langle\mathbf{E}\mathbf{E}\rangle\right]$$

Maxwell tensor

- **Collisional absorption:**
  - Poynting theorem: $\nabla\cdot\mathbf{S} = -\mathbf{j}\cdot\mathbf{E}$

Poynting vector

  - Time-average: $W_L = \langle \mathbf{j}\cdot\mathbf{E}\rangle = -\nabla\cdot\langle\mathbf{S}\rangle$

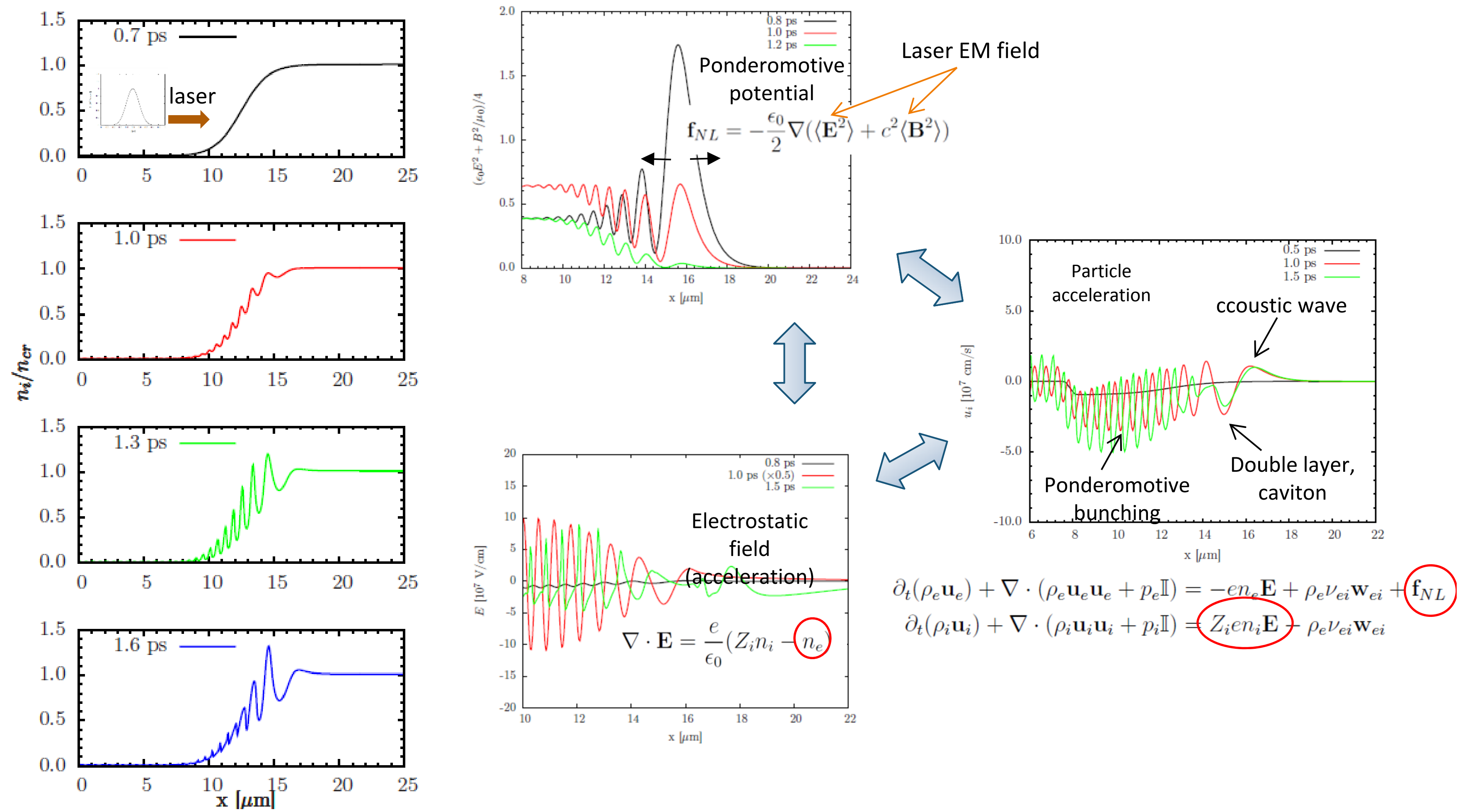


- **Assume 1-d propagation:**

$$\mathbf{f}_p = -\frac{\epsilon_0\omega_p^2}{4\omega^2}\partial_x\left(\hat{\mathbf{E}}\hat{\mathbf{E}}^\star\right)$$

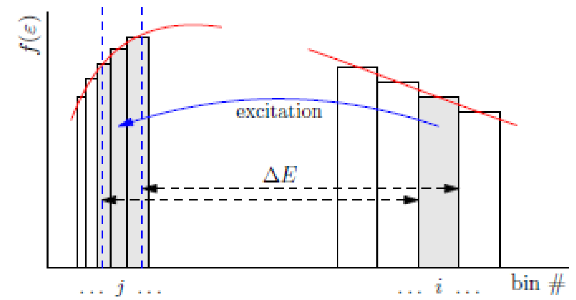
Laser-Plasma Interaction

- **Ion acceleration due to ponderomotive force**



Beyond Maxwellian: Kn = O(1)

- **Not-too-far from equilibrium (isotropic)**
  - Discretized EEDF yields rate equations for discrete elements ("bin")
  - DB enforced at microscopic level
  - High-order, implicit and energy conserving
  - More efficient compared to MCC.
- **Far from equilibrium**
  - MCC algorithm for inelastic collisions
  - Can resolve anisotropic vdf
  - Drawback: slow convergence, reaction branching, singular rates, computational particle growth



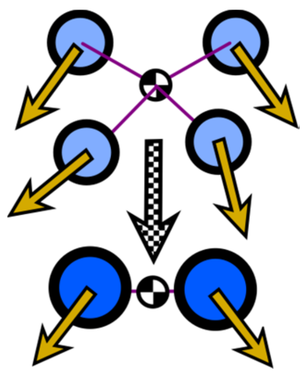
$$\bar{n}_i = N_e \int_{\varepsilon_i}^{\varepsilon_i+\Delta\varepsilon} d\varepsilon\, f_e(\varepsilon)$$

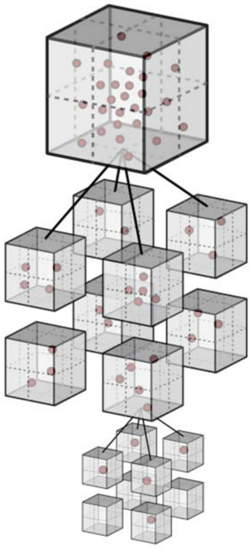
$$\frac{d\bar{n}_i}{dt} = -N_l\,\bar{n}_i \sum_j \bar{k}^{\mathrm{exc}}_{(j|i)} + N_u \sum_j \bar{n}_j \bar{k}^{\mathrm{dex}}_{(i|j)}$$

$$\frac{d\bar{n}_j}{dt} = +N_l \sum_i \bar{n}_i \bar{k}^{\mathrm{exc}}_{(j|i)} - N_u\,\bar{n}_j \sum_i \bar{k}^{\mathrm{dex}}_{(i|j)}$$

Beyond Maxwellian: Particle Merging

- Scheme built on merging 3+ particles to 2.
- Mass, momentum and kinetic energy are exactly conserved; Electrostatic energy also conserved in physical space.
- Split analogously defined by merging only fractions of original particles.
- Octree in velocity space inhibits thermalization by ensuring only near neighbor particles are merged.
- Higher-moment conserving schemes have been obtained with increased number of merge result particles generated.



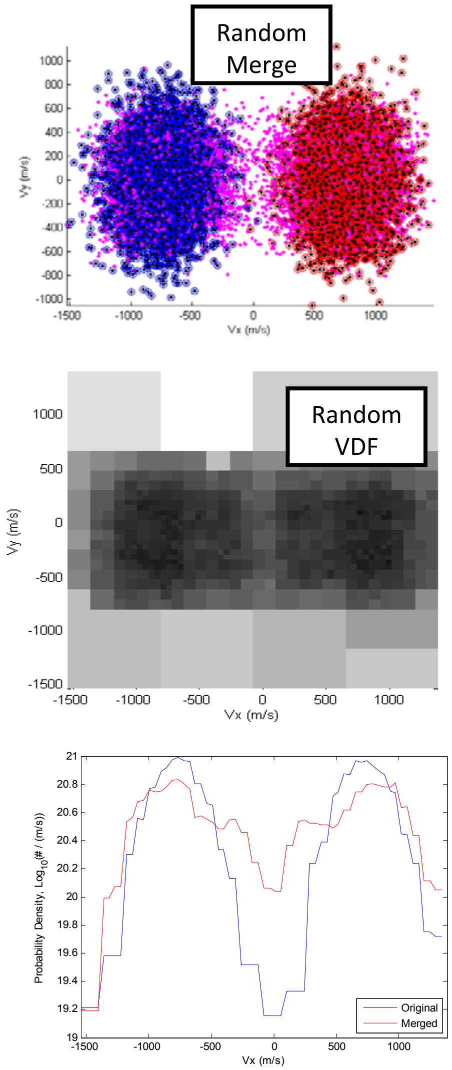


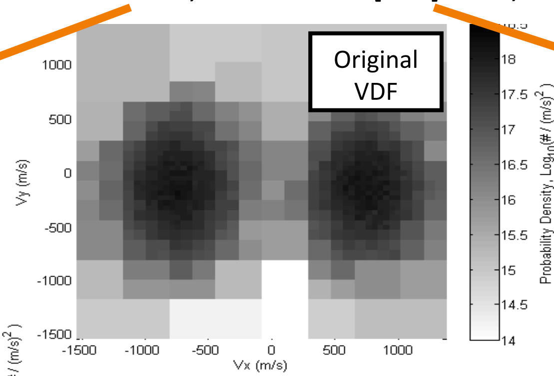
Particle Merge: Importance of Octree

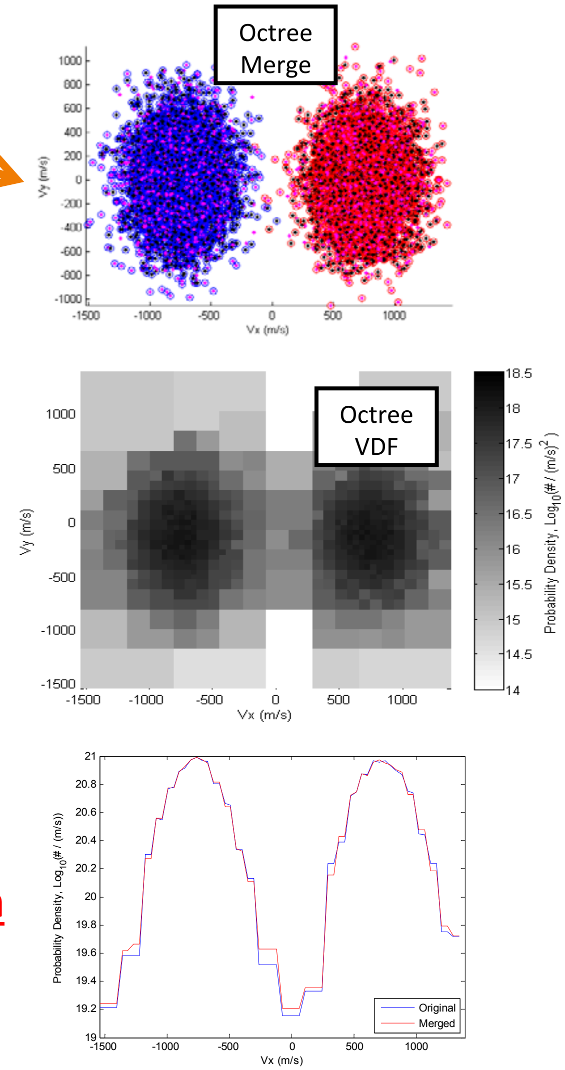
Original ---10,000 Particles

Random 4:2 → 5,000

Octree [3-11]:2 → 4,727







Mass/Momentum/Energy Conserving Merge for Both

Energy Conserved

-But-

Entropy Unequal

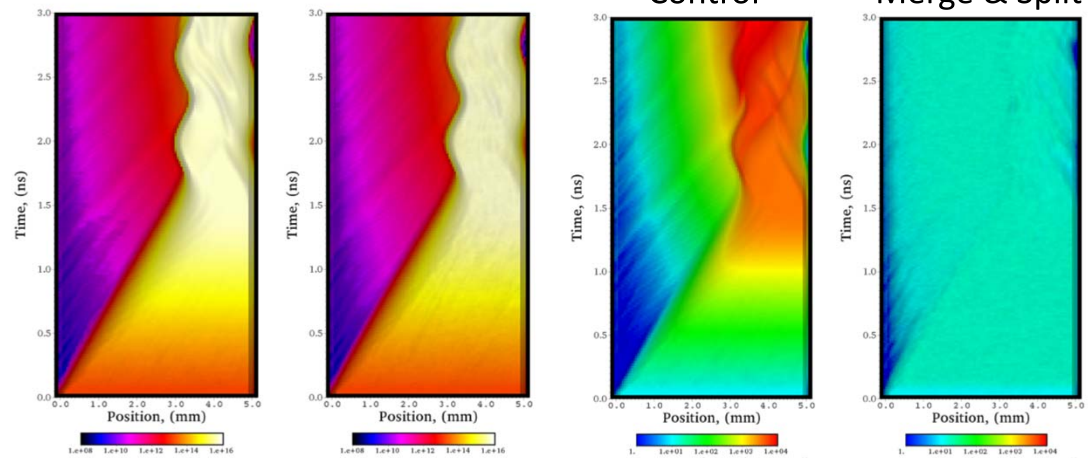
Octree VDF Shape Preservation Inhibits Thermalization

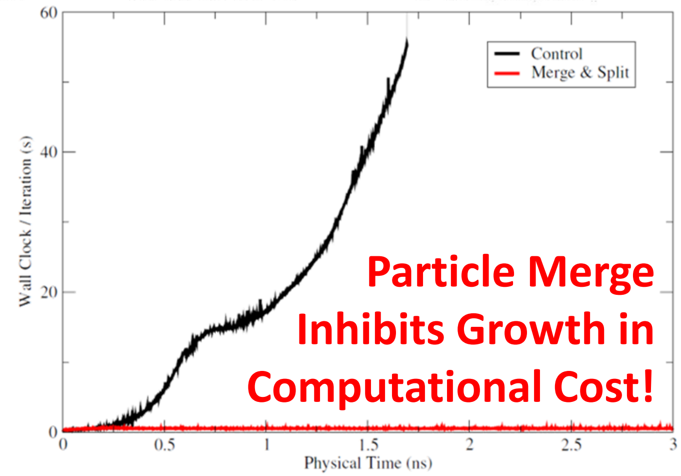
Particle Merge: DC Breakdown Case

- Tested in 3D ES-PIC of 1-KV DC Breakdown
- MCC-Ionization, Chain Branching & Cathode Secondary Emission causes exponential growth in cost
- With Merging: Density matches despite vastly different number of Computational Particles/Cell
- Negligible overheard demonstrated in comparison of wall-clock/iteration with merge every iteration
- Enables direct control of computational cost in particle methods
- Future Work: Test merge in non-Maxwellian laser plasma test case

Density | Computational Particles/Cell

Control | Merge & Split | Control | Merge & Split





Conclusion

- **Multiscale algorithms for nonequilibrium flows with CR kinetics**
  - Level grouping schemes of electronic states of atoms.
  - Multi-fluid equations developed to efficiently capture electron "hydrodynamics"
  - Particle merge/split for particle management, efficient sampling, inelastic collisions …
- **Ongoing works:**
  - Multi-D simulation with level grouping
  - Modeling of inelastic collisions in multi-fluid
  - High-order particle merging schemes